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Effect of interface/surface stress on the elastic wave band structure of two-dimensional phononic crystals

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ABSTRACT

In the present Letter, the multiple scattering theory (MST) for calculating the elastic wave band structure of two-dimensional phononic crystals (PCs) is extended to include the interface/surface stress effect at the nanoscale. The interface/surface elasticity theory is employed to describe the nonclassical boundary conditions at the interface/surface and the elastic Mie scattering matrix embodying the interface/surface stress effect is derived. Using this extended MST, the authors investigate the interface/surface stress effect on the elastic wave band structure of two-dimensional PCs, which is demonstrated to be significant when the characteristic size reduces to nanometers.

1. Introduction

Propagation of elastic waves in artificial periodic composites, termed as phononic crystals (PCs), has received increasing research attention in recent years [1–6]. The existence of band gaps, i.e. frequency ranges within which propagation of elastic waves is completely forbidden inside the crystals, has been predicted theoretically [1–4] and demonstrated experimentally [5,6]. PCs have also been found to posses some peculiar properties under certain conditions, e.g. negative refraction and sound focusing [7,8], subwavelength imaging [9–12] and collimation [13–17]. Therefore, various applications of PCs have been expected, for example, sound insulators, filters and waveguides. The identification of band gaps and frequency regimes where the aforementioned unique properties may occur relies on the band structure calculation results. Up to now, several methods have been proposed for calculating the elastic wave band structure of PCs, including the plane wave expansion (PWE) method [1,3,4], the finite difference time domain (FDTD) method [18,19], and the multiple scattering theory (MST) method [20–22].

Recently, the possibility of fabricating and measuring micro and nano PCs [23,24] have been demonstrated and the integration of devices based on PCs into communication and sensing systems has been anticipated in pace with the development of nanotechnologies. It has long been known that interface/surface stress may have significant effect on the mechanical and other physical behaviors of smallsized materials and structures due to the high interface/surface-to-volume ratio [25–27]. Gurtin and Murdoch [28] and Gurtin et al. [29] developed the interface/surface elasticity theory to describe the interface/surface stress effect in the continuum framework and the interface/surface elasticity theory has been demonstrated to be capable of well reproducing the results of direct atomic simulations [27]. The interface/surface elasticity theory has been employed to study the size-dependent effective elastic constants of solids containing nano-inhomogeneities [30]. Some authors have investigated and demonstrated the interface/surface stress effect on the wave propagation in solids. Gurtin and Murdoch [31] investigated the effect of surface stress on plane wave propagation in homogeneous, isotropic half spaces. Wang [32] and Wang et al. [33,34] studied the diffraction of plane elastic waves by nanosized inhomogeneities and demonstrated the considerable importance of the interface/surface stress effect.

To date, little attention has been paid to the interface/surface stress effect on the wave propagation in PCs, which is of importance for designing and characterizing miniaturized devices based on PCs. In this Letter, we extend the MST by incorporating the interface/surface elasticity theory and investigate the interface/surface stress effect on the elastic wave band structure of two-dimensional PCs.

2. Basic equations of interface/surface elasticity

According to the interface/surface elasticity theory, the interface/surface is viewed as a negligibly thin elastic continuum which adheres to the bulk materials without slipping. The elastic constants of the interface/surface are different from those of the bulk

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materials. Assume a coherent interface Γ between two different solids Ω_1 and Ω_2. The equilibrium equation of the interface Γ takes the following form [28,30]

$$\left(\boldsymbol{\sigma}^1 - \boldsymbol{\sigma}^2\right) \cdot \mathbf{n} = -\nabla_s \cdot \boldsymbol{\tau} \tag{1}$$

where $\boldsymbol{\sigma}^1$ and $\boldsymbol{\sigma}^2$ are the stress tensor in solids Ω_1 and Ω_2, respectively, and $\mathbf{n}$ denotes the unit normal vector to the interface Γ, with positive $\mathbf{n}$ being from Ω_2 to Ω_1. $\nabla_s \cdot \boldsymbol{\tau}$ denotes the interface/surface divergence of the interface/surface stress $\boldsymbol{\tau}$.

For a linear elastically isotropic interface/surface, the constitutive equation reads [27,30,32]

$$\boldsymbol{\tau} = \lambda_s \left(\operatorname{tr} \boldsymbol{\varepsilon}^s\right)\mathbf{I} + 2\mu_s \boldsymbol{\varepsilon}^s \tag{2}$$

where λ_s and μ_s are the interface/surface elastic moduli, and $\mathbf{I}$ is the second-rank unit tensor in two-dimensional space. $\boldsymbol{\varepsilon}^s$ is the second-rank tensor of interface/surface strains, which for a coherent interface/surface equals to the tangential strain of the bulk materials at the interface/surface.

The equilibrium equations, constitutive equations and the strain-displacement equations in the bulk materials are the same as those of classical elasticity.

3. MST with interface/surface stress effect taken into account

3.1. Fundamentals of MST

The MST has already been successfully applied to calculating the band structure of various PCs [20–22] and it features excellent convergence and capability of handling PCs with mixing solid and fluid components. Compared with the other methods, the MST explicitly utilizes the boundary conditions at the interface/surface, and thus offers the potential to conveniently embody the interface/surface stress effect. Based on the interface/surface elasticity, here we extend the MST and investigate the interface/surface stress effect on the elastic wave band structure of 2D PCs. To be complete, the fundamentals of the MST are outlined in this section.

Consider two-dimensional PCs consisting of aligned cylindrical inclusions or pores periodically embedded in a matrix. The time-harmonic elastic wave equation in linear, isotropic, homogeneous media reads

$$(\lambda + 2\mu)\nabla\nabla \cdot \mathbf{u} - \mu\nabla \times \nabla \times \mathbf{u} + \rho\omega^2\mathbf{u} = 0 \tag{3}$$

where $\mathbf{u}$ is the displacement, λ and μ the Lamé constants, and ρ the mass density of the medium. In the cylindrical coordinate system (r, ϕ, z), the general solution of Eq. (3) is of the following form [22]

$$\mathbf{u}(\mathbf{r}) = \sum_{n\zeta} \left[a_{n\zeta}\mathbf{J}_{n\zeta}(\mathbf{r}) + b_{n\zeta}\mathbf{H}_{n\zeta}(\mathbf{r})\right] \tag{4}$$

where $\mathbf{J}_{n\zeta}(\mathbf{r})$ and $\mathbf{H}_{n\zeta}(\mathbf{r})$ are defined as [22]

$$\begin{aligned}
\mathbf{J}_{n1}(\mathbf{r}) &= \nabla\left[J_n(\alpha r)e^{in\phi}\right] \\
\mathbf{J}_{n2}(\mathbf{r}) &= \nabla \times \left[\mathbf{z}J_n(\beta r)e^{in\phi}\right] \\
\mathbf{J}_{n3}(\mathbf{r}) &= \frac{1}{\beta}\nabla \times \nabla \times \left[\mathbf{z}J_n(\beta r)e^{in\phi}\right]
\end{aligned} \tag{5}$$

and

$$\begin{aligned}
\mathbf{H}_{n1}(\mathbf{r}) &= \nabla\left[H_n(\alpha r)e^{in\phi}\right] \\
\mathbf{H}_{n2}(\mathbf{r}) &= \nabla \times \left[\mathbf{z}H_n(\beta r)e^{in\phi}\right] \\
\mathbf{H}_{n3}(\mathbf{r}) &= \frac{1}{\beta}\nabla \times \nabla \times \left[\mathbf{z}H_n(\beta r)e^{in\phi}\right]
\end{aligned} \tag{6}$$

where $\alpha = \omega\sqrt{\rho/(\lambda + 2\mu)}$, $\beta = \omega\sqrt{\rho/\mu}$, $J_n(x)$ is the Bessel function, and $H_n(x)$ is the Hankel function of the first kind. The index ζ in Eq. (4), running from 1 to 3, represents three wave modes, i.e. the longitudinal mode ($\zeta = 1$) and the two shear modes ($\zeta = 2, 3$). The first and second term of the right-hand side of Eq. (4) stand for the incoming and outgoing waves, respectively.

According to the MST, in a multiple scattering system, the incident wave at each scatterer N located at the lattice position $\mathbf{R}_N$, $\mathbf{u}_N^{inc}$, is equal to the sum of the scattered waves from all the other scatterers plus the possible external incident wave $\mathbf{u}^{inc(0)}$. This physical picture can be mathematically expressed as

$$\mathbf{u}_N^{inc}(\mathbf{r}_N) = \mathbf{u}^{inc(0)}(\mathbf{r}_N) + \sum_{M \neq N} \mathbf{u}_M^{sc}(\mathbf{r}_M) \tag{7}$$

where $\mathbf{r}_N$ and $\mathbf{r}_M$ denote the position of the same spatial point measured from scatterers N and M, respectively. Using the general solution in Eq. (4), Eq. (7) can be recast into the following form

$$\begin{aligned}
&\sum_{n\zeta} a_{n\zeta}^N \mathbf{J}_{n\zeta}(\mathbf{r}_N) \\
&\quad = \sum_{n'\zeta'} a_{n'\zeta'}^{N(0)} \mathbf{J}_{n'\zeta'}(\mathbf{r}_N) + \sum_{M \neq N} \sum_{n''\zeta''} b_{n''\zeta''}^M \mathbf{H}_{n''\zeta''}(\mathbf{r}_M)
\end{aligned} \tag{8}$$

The scattered wave by each scatterer can be related to the incident wave at the same scatterer by the following relation between the incident field expansion coefficients $\mathbf{A} = \{a_{n\zeta}^N\}$ and the scattered field expansion coefficients $\mathbf{B} = \{b_{n\zeta}^N\}$:

$$\mathbf{B} = \mathbf{TA} \tag{9}$$

where the elastic Mie scattering matrix $\mathbf{T} = \{t_{n\zeta n'\zeta'}\}$ can be obtained from the boundary conditions at the interface/surface. For PCs consisting of identical scatterers, $\mathbf{T}$ is independent of the lattice position.

The scattered field from scatterer M can be translated to the incident field at scatterer N by using the following relation [22]

$$\mathbf{H}_{n\zeta}(\mathbf{r}_M) = \sum_{n'\zeta'} G_{n\zeta n'\zeta'}(\mathbf{R}_M - \mathbf{R}_N)\mathbf{J}_{n'\zeta'}(\mathbf{r}_N) \tag{10}$$

where $G_{n\zeta n'\zeta'}(\mathbf{R}_M - \mathbf{R}_N)$ is given by

$$G_{n\zeta n'\zeta'}(\mathbf{R}) = \begin{cases} H_{n'-n}(\alpha R)e^{-i(n'-n)\phi_R}, & \zeta = \zeta' = 1 \\ H_{n'-n}(\beta R)e^{-i(n'-n)\phi_R}, & \zeta = \zeta' = 2, 3 \end{cases} \tag{11}$$

In addition, by using Bloch's theorem one can relate the expansion coefficients $a_{n\zeta}$ at different lattice positions

$$a_{n\zeta}^M = e^{i\mathbf{k}\cdot(\mathbf{R}_M - \mathbf{R}_N)} a_{n\zeta}^N \tag{12}$$

where $\mathbf{k}$ is the Bloch wave vector. Since the elastic wave band structure is concerned, the external incident wave in Eq. (8) vanishes. Substituting Eqs. (9)–(12) into Eq. (8) yields

$$\begin{aligned}
&\sum_{n'\zeta'} \left[\sum_{n''\zeta''} t_{n''\zeta''n'\zeta'} \sum_{M \neq N} e^{i\mathbf{k}\cdot(\mathbf{R}_M - \mathbf{R}_N)} G_{n''\zeta''n\zeta}(\mathbf{R}_M - \mathbf{R}_N) - \delta_{nn'}\delta_{\zeta\zeta'}\right] \\
&\quad \times a_{n'\zeta'}^N = 0
\end{aligned} \tag{13}$$

where δ is the Kronecker delta, and thus the elastic wave band structure of 2D PCs can be obtained by solving the following secular equation

$$\det\left|\sum_{n''\zeta''} t_{n''\zeta''n'\zeta'} g_{n''\zeta''n\zeta}(\mathbf{k}) - \delta_{nn'}\delta_{\zeta\zeta'}\right| = 0 \tag{14}$$